



Combinatorial Methodologies for Advanced Materials: An ATP Workshop

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http://www.atp.nist.gov/www/ccmr/ccmr_off.htm



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Workshop Agenda

- 08:30 – 08:45 John Hewes (ATP) Workshop Kick-off
- 08:45 – 09:15 Peter Cohan (Symyx) "Implementation Issues"
- 09:15 – 09:30 Richard Morris (ATP) "Software Issues for Combinatorial Methods"
- 09:30 – 10:00 Doug Lenat (Cycorp) "Artificial Intelligence--Thesauri"
- 10:00 - 10:15 Break**
- 10:15 - 10:45 Andrew Canning (LBNL): "Teraflop Computing for Advanced Materials"
- 10:45 - 11:15 David Dorsett (Symyx) "Datamining"
- 11:15 - 11:45 Rock Gnatovich, Spotfire "Visualization Tools"
- 11:45 – 12:15 Participant Discussion of Software Issues for Combinatorial Methods
- 12:15 – 13:30 Informal Lunch Discussion**
- 13:30 – 13:45 John Hewes (ATP) "Hardware Issues for Combinatorial Methods"
- 13:45 – 14:15 Jim Cawse (GE CR&D) "Six Sigma in Combinatorial Methods"
- 14:15 - 14:45 MaryAnn Asaro (SRI) "Advances in Combinatorial Chemistry"
- 14:45 – 15:15 Pam York (Sarnoff) "Challenges in Lab-on-chip Technologies"
- 15:15 - 15:30 Break**
- 15:30 – 16:00 Joseph Hogan (Alveus Systems) "Advances in Combinatorial Chemistry"
- 16:00 – 16:30 Selim Senkan (UCLA) "Combi Methods for Heterogeneous Catalysts"
- 16:30 – 17:00 Al Sylwester (Sandia) "Sandia's Micro Lab-on-Chip"
- 17:00 – 17:30 John Hewes (ATP) "Workshop Wrap-up"



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Part I: Welcome and Introduction



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What ATP Looks For...

ATP Cost-Shares High Risk, Enabling Technology

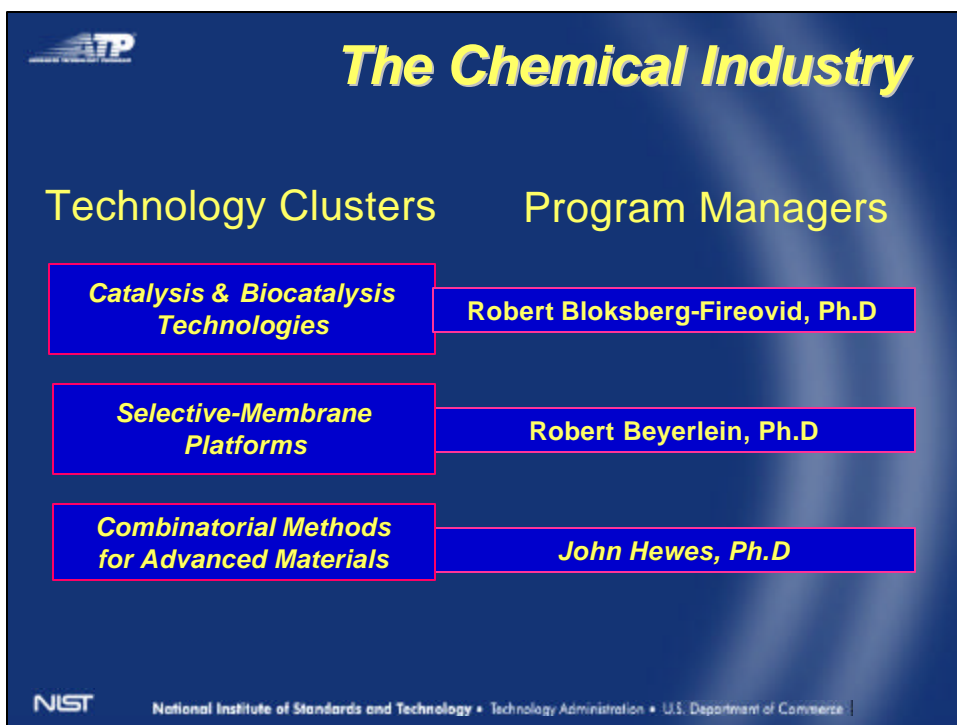
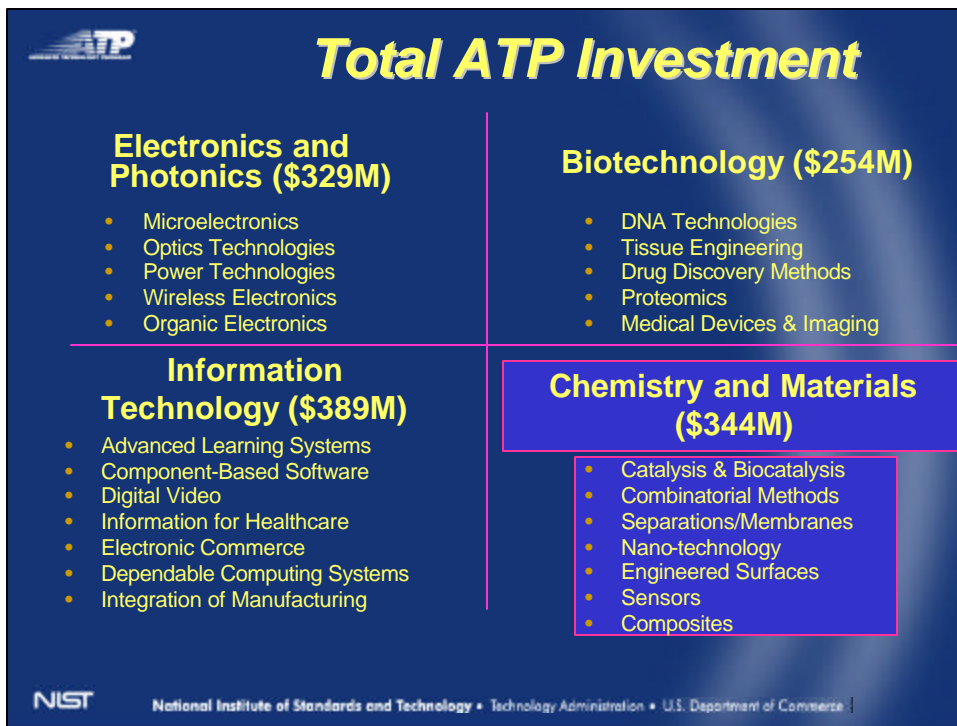
- Path-breaking technology
 - ✓ *Opens up new possibilities*
 - ✓ *Revolutionary in nature*
- Infrastructural technology
 - ✓ *Supports an entire industry*
- Multi-use technology
 - ✓ *Many distinct applications*

ATP Ground Rules:

- Confidential reviews by Federal employees
- Companies retain patent rights
- Projects in *all* technology areas are supported



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ATP Technology Cluster

*Combinatorial Methods for Advanced Materials R&D
FY 1999 Projects: \$23M from ATP over 5 years*

Nonlinear Dynamics/UOP LLP	"Combinatorial Tools and Advanced Data Analysis Methods for Heterogeneous Catalysts" \$14,715K (ATP) + \$15,186 (j/v) (5 yrs.)
GE/Avery-Dennison	"Combinatorial Methodology for Coatings Development" \$3,127K (ATP) + \$3,200K (j/v) (3 yrs.)
Catalytica/CombiChem/Exxon	"A Strategy for Reclaiming U.S. Leadership in High Value Polymers (Polyolefins)" \$4,861K (ATP) + \$6,049K (j/v) (3 yrs.)

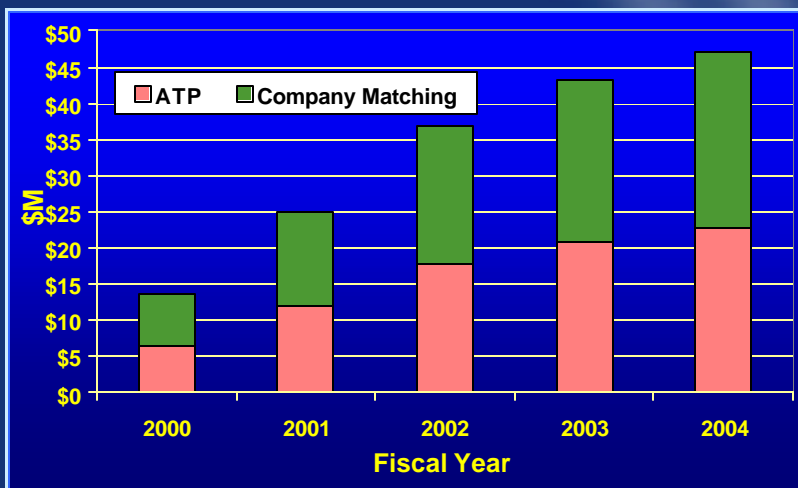


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ATP Combi Methods Cluster

Cumulative Project Expenditures, 1999 - 2004



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Industry Drivers-Combi

- **Reduced innovation cycle times across organization**
 - ✓ *Discovery*
 - ✓ *Process and product development*
 - ✓ *Customer service and manufacturing*
- **More efficient use of capital for R&D and manufacturing**
 - ✓ *Time-to-market and ROI of R&D \$'s*
- **New products/new technologies = new markets**
- **Allows for “out-of-box” experimentation**
 - ✓ *Broadens spectrum of materials in development*



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Competitive Threats

- Reverse engineering of intellectual property
- First-to-market, first-to-follow market positioning
- Faster response to customer needs
- Lower R&D cost structures, higher-performance
- Leverage of government funding

New compositions, faster, at lower R&D cost



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Why Combi Methods Now?

- *Strategic Inflection Points*
- *Horizontal Integration of computers & electronics*
 - *A. Groves, Only the Paranoid Survive*

*The New SIP: Outsourcing of Discovery, Lean R&D,
Horizontal Distribution of Knowledge Capital*



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Why ATP?

- Stimulate convergence of technologies
- Focused infrastructure development toward specific advanced materials applications
- Leverage leading-edge capabilities to lower-margin, less R&D-intensive industries than pharma
 - ✓ *Timing is critical*
 - ✓ *Benefits firms of all sizes, with many alliances possible*
 - ✓ *Multi-Skill Center effort (broad synergies)*
 - ✓ *New tools for research and development*
 - ✓ *Large spill-over benefits to/from basic science*

ATP can help U.S. industry implement!



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Plan Forward—FY '00

Chemical/Materials industry identified two challenges for
Discovery and Product & Process Development Processes

Informatics

- Design of the Library
 - ✓ Computational/Modeling: QSPR
 - ✓ Statistics and control of error
 - ✓ Design of Experiments
- Informatics
 - ✓ Increasing Information/Bandwidth
 - ✓ Experimental complexity
 - ✓ Data integration/analysis
 - ✓ Hardware control
 - ✓ Expert systems for data analysis

Micro-Characterization

- Screening
 - ✓ MEMS: Lab-on-chip, Sensors
 - ✓ Deposition/library fabrication
 - ✓ Process control
 - Temperature/pressure
 - ✓ Scalability Predictions
 - Interfacial properties
- Synthesis and Processing
 - ✓ Automation: 10^3 - 10^4 samples
 - ✓ Reproducibility
 - ✓ Validation



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Part II: Characterization Issues



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Enabling Technologies

Design

- Literature/Patent Data mining as input to library design
- Statistics, modeling, design of experiments
- Diversity analysis/clustering analysis
- Computational: Molecular Modeling, QSAR, QSPR

Fabrication

- Chemical/Physical/Plasma Deposition
- Ink jet
- Thermally-driven deposition (e-beam, LEED, etc.)
- Laser ablation

Characterization

- Sample size --understanding interfacial properties, diffusion, mass transport at micro-scale
- Mechanical and physical properties
- Error Identification On-line/Validation

Informatics

- Data Mining, connectivity, parallelism, registration, ...

Systems Integration is a Significant Challenge



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Target Applications-Combi

Catalysts

Electronic Materials

Polymers/Chemicals
Phosphors
Magnetic Materials
Ceramics
Semiconductors

Polymers

Membranes
Encapsulants/packaging
Adhesives
Coatings

Biomaterials

Bio-sourced polymers
Bio-compatible materials
Bio-degradable polymers

Optical materials

Coatings
Photo-refractives
Opto-electronics
Non-Linear Optical materials

Structural materials

Metals and alloys
Composites
Ceramics/metal oxides

Glasses

Fibers
Electronic
Magnetic
Optical

Smart Materials

Advanced Ceramics

Specialty
Optical & Electronic
Super-conducting
Structural
Coatings

Profit Margin, R&D Budget, and Cost/Benefit Define Combi Entry



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Drug Discovery

- Discrete molecules of C, H, F, N, O, P
- Finite number of active sites, can be characterized and modeled computationally
- Synthesis usually leads to substances of >85% purity; parallel purification techniques employed before characterization
- Structures reproducible (*a priori*)
- Chemical characterization, biological activity well developed for rapid or parallel, methods
- Descriptors for diversity
- Registration of library samples straightforward
- Synthetic building blocks available

Solid State Materials

- Extended structures of many elements potentially in metastable states
- Ill-defined distribution of active sites and structures
- "Pure" solids are meaningless especially with small samples having interfacial effects with the library substrate
- Reproducible structures hard, if not impossible, to create *a priori*
- Characterization of properties and composition not straightforward
- No ideas exist about how to do it
- No ideas exist about how to do it
- A few building blocks available



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Issues--Characterization

- Miniaturization/parallelization of reaction, processing, and testing apparatus
- Micro-sensors (*in situ* analysis)
- High-level Integration
- Clear understanding of "scalability"
 - ✓ Validation of micro- vs. bulk properties
- Deposition of samples
 - ✓ Ink jet, PVD, CVD, etc.....



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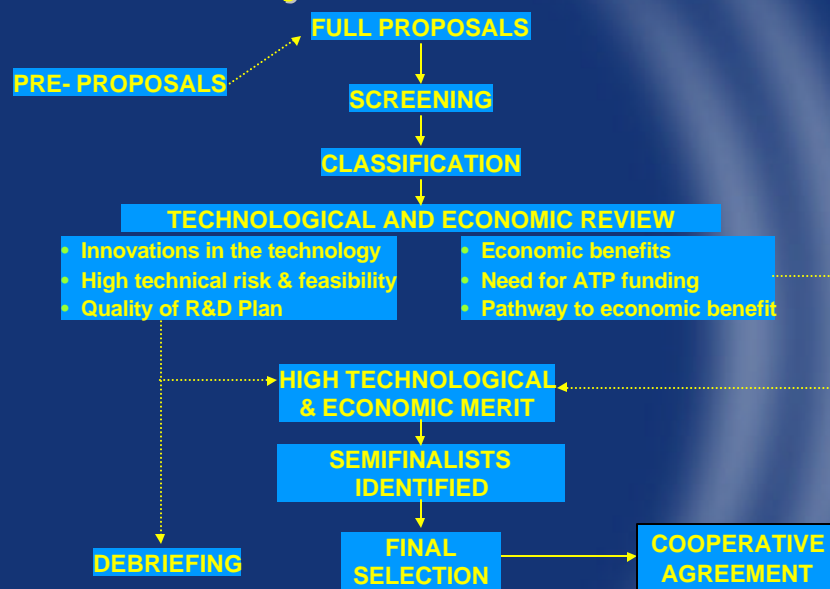
Part III: Proposals



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Project Selection Process



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Rules for Participation ...

- Must produce U.S. economic benefits
 - ✓ R&D and manufacturing in the U.S.
 - ✓ Increase U.S. employment
 - ✓ Promote U.S. supplier infrastructure
- Companies incorporated in the U.S.
- Keep intellectual property rights
- Confidentiality (not subject to FOIA)
- Universities and non-profit research organizations may receive share of return from royalties but cannot own title to intellectual property



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How to apply

- Pre-proposals--Year-round submission
- Full Proposals—Annual Competition
 - ✓ *Announced late Fall, due early Spring*
- Obtain and **read** the Preparation Kit
 - ✓ *Hardcopy, online or CD-ROM*
- Assemble Proposal
 - ✓ *Commercialization **and** Technical Plans are evaluated by experts for feasibility*
 - ✓ Multi-functional team highly recommended

Most Common Error is Lack of Detail in Proposal



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Critical Proposal Elements

- **Scientific and Technological Merit (50%)**

- ✓ Innovations in the Technology
- ✓ High Technical Risk & Feasibility
- ✓ Quality of R&D Plan



- **Broad-Based Economic Benefits (50%)**

- ✓ Economic Benefits
- ✓ Need for ATP Funding
- ✓ Pathway to Economic Benefits



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Common Weaknesses

- Proposals lack of sufficient detail for peer review
 - ✓ *How you will reach technical objectives*
 - ✓ *What's innovative about the approach*
 - ✓ *Why a risky technical approach is needed*
- Proposals have unsupported assertions that project meets ATP's criteria
- Proposals miss ATP's window of opportunity
 - ✓ *Low risk - product development (too late)*
 - ✓ *Lacks demonstrated feasibility (too early)*



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Some helpful hints ...

- Proposals due at **3:00 p.m. (Eastern)** on the specified date -- ***no fax or electronic transmittal***
- Late proposals rejected. ***NO EXCEPTIONS!***
- Overnight mail companies sometimes *don't* deliver overnight
- Send your proposal in early
- **Read the Proposal Prep Kit**



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Contact Information

www.atp.nist.gov

To Get on the ATP Mailing List:

Call toll-free: 800-ATP-FUND
(800-287-3863)

Fax your name and address to: (301) 926-9524

Send an e-mail message to: atp@nist.gov



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